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Numerical Computation of Exponential Matrices Using the Cayley-Hamilton Theorem

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ABSTRACT

A method for computing exponential matrices, which often arise naturally in the solution of systems of linear differential equations, is developed. An exponential matrix is generated as a linear combination of a finite number (equal to the matrix order) of matrices, the coefficients of which are scalar infinite sums. The method can be generalized to apply to any formal power series of matrices. In this paper, attention is focused upon the exponential function, and the matrix exponent is assumed tri-diagonal in form. In such case, the terms in the coefficient infinite sums can be extracted, as recursion relations, from the characteristic polynomial of the matrix exponent. Two numerical examples are presented in some detail: (1) the three-dimensional infinitesimal rotation rate matrix, which is skew-symmetric, and (2) an N-dimensional tri-diagonal and symmetric finite difference matrix which arises in the numerical solution of the heat conduction partial differential equation. In the second example, the known eigenvalues and eigenvectors of the finite difference matrix permit an analytical solution for the exponential matrix, through the theory of diagonalization and similarity transformations, which is used for independent verification. The convergence properties of the scalar infinite summations are investigated

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for finite difference matrices of various orders up to ten, and it is found that the number of terms required for convergence increases slowly with the order of the matrix. Successive squarings of the exponential matrix demonstrate that the resultant limiting matrix tends toward zero in a smooth fashion, due to the dominance of the largest eigenvalue of the finite difference matrix. An appendix to the paper presents an algorithm for the evaluation of exponential matrices.

NUMERICAL COMPUTATION OF EXPONENTIAL MATRICES
USING THE CAYLEY-HAMILTON THEOREM

INTRODUCTION

The concept of exponential matrix arises naturally in physical problems in which the underlying (possibly high-order) differential equations can be reduced to a system of linear differential equations. In the simplest case, the fundamental solution y(x) of the linear differential equation $dy/dx = Ay$, where A is a scalar constant, is given by:

$$y(x) = y(0)\, e^{Ax} = y(0) \sum_{k=0}^{\infty} \frac{1}{k!} A^k x^k .$$

When y is a vector and A is a square matrix, then the infinite series of matrices given above is still well defined, i.e., converges uniformly and absolutely for x in any bounded interval [1, pp. 64-65], and provides the solution to the linear differential equation in terms of the exponential matrix, exp (Ax).

As an example of a physical problem in which exponential matrices arise, consider the representation of the propagation operator for energetic charged particles in the interplanetary magnetic field. The propagation equation, a second-order partial differential equation with three independent variables, may be reduced, under appropriate assumptions, to a steady-state relation with only two independent variables. This steady-state second-order partial differential equation may be solved by finite-difference methods using discrete ordinates, in which the second-order partial differential operator is replaced by a second-order difference operator represented by a matrix M, which is tri-diagonal in form. The propagation equation may thus be written as

$$\frac{\partial W_i}{\partial s'} = \sum_{j=1}^{N} M_{ij}\, W_j ,$$

whose solution may be expressed in terms of an exponential matrix:

$$W(s') = W(0)\, e^{Ms'} \equiv W(0) \sum_{k=0}^{\infty} \frac{1}{k!} M^k (s')^k .$$

A method for generating such an exponential matrix as a linear combination of a finite number N of matrices will be discussed in this paper.

POWER SERIES OF MATRICES

According to the Cayley-Hamilton theorem [1, p. 113], a square matrix satisfies its own characteristic equation. For an N x N matrix M, let the characteristic polynomial be written as

$$p^N(\lambda) = \det(\lambda I_N - M) = \sum_{n=0}^{N} a_n^N \lambda^n , \tag{1}$$

where the coefficient $a_N^N = 1$, and I_N is the N x N identity matrix. Thus, by the Cayley-Hamilton theorem, $p^N(M) = 0$, or

$$M^N = -\sum_{n=0}^{N-1} a_n^N M^n . \tag{2}$$

This relationship leads to the conclusion that any positive integral power of M can be expressed as a linear combination of the N matrices, $I_N, M, M^2, \ldots, M^{N-1}$. In fact, when the inverse M^{-1} exists, the preceding statement may be generalized to any integral power. Suppose this is true for some integral power k, so that

$$M^k = -\sum_{n=0}^{N-1} A_n^k M^n , \tag{3}$$

where the A_n^k are suitably chosen scalar coefficients. Then, multiplying by M, one finds

$$M^{k+1} = -\sum_{n=1}^{N-1} A_{n-1}^k M^n - A_{N-1}^k M^N . \tag{4}$$

Substituting for M^N from equation (2),

$$M^{k+1} = \sum_{n=1}^{N-1} (A_{N-1}^{k}\, a_n^N - A_{n-1}^{k})\, M^n + A_{N-1}^{k}\, a_o^N\, I_N \,, \tag{5}$$

whereas equation (3) for k+1 yields

$$M^{k+1} = -\sum_{n=1}^{N-1} A_n^{k+1}\, M^n - A_o^{k+1}\, I_N \,. \tag{6}$$

Equating coefficients of equal powers of M in equations (5) and (6) results in the recursion relationships:

$$A_n^{k+1} = A_{n-1}^{k} - A_{N-1}^{k}\, a_n^N, \quad \text{for } 1 \leqslant n \leqslant N-1, \tag{7a}$$

$$A_o^{k+1} = -A_{N-1}^{k}\, a_o^N \,. \tag{7b}$$

If we establish the convention $A_{-1}^{k} \equiv 0$, then the above relations combine to

$$A_n^{k+1} = A_{n-1}^{k} - A_{N-1}^{k}\, a_n^N, \quad \text{for } 0 \leqslant n \leqslant N-1 \,. \tag{8}$$

By comparing equation (2) with equation (3) for k = N, we find

$$A_n^N = a_n^N \,, \quad \text{for } 0 \leqslant n \leqslant N-1 \,. \tag{9}$$

In what follows, we shall assume that $k \geqslant N$ in equation (8) and extend the range of the indices of A_n^k by defining (in terms of the Kronecker delta)

$$A_n^k = -\,\delta_{kn} \,, \quad \text{for } 0 \leqslant k \leqslant N-1 \,. \tag{10}$$

Any formal power series f(M) derived from the infinite expansion,

$$f(X) = \sum_{k=0}^{\infty} B_k\, X^k \,, \tag{11}$$

can be expressed as a linear combination of the N matrices, I_N, M, M^2, . . ., M^{N-1}, in the form

$$f(M) = \sum_{k=0}^{\infty} B_k M^k = - \sum_{k=0}^{\infty} B_k \sum_{n=0}^{N-1} A_n^k M^n \tag{12a}$$

$$= - \sum_{n=0}^{N-1} \left(\sum_{k=0}^{\infty} B_k A_n^k \right) M^n , \tag{12b}$$

upon substitution of equation (3) and interchanging the order of the summations. Note that evaluation of f(M) in this manner requires only N scalar infinite sums as coefficients of the matrices.

A typical power series might be the exponential function $f(X) = e^X$ for which $B_k = 1/k!$. In this case, the sequence B_k is rapidly converging toward zero, and, in order to overcome possible numerical difficulties in a situation in which the coefficients A_n^k are diverging as $k \to \infty$, we may define a new well-bounded sequence

$$C_n^k \equiv B_k A_n^k = \frac{A_n^k}{k!} . \tag{13}$$

For this power series, equation (12b) may be written

$$e^M = - \sum_{n=0}^{N-1} \left(\sum_{k=0}^{\infty} C_n^k \right) M^n , \tag{14}$$

in which the left side is an exponential matrix. The recursion relation (8), upon multiplication by B_{k+1}, may be rewritten as

$$C_n^{k+1} = \frac{1}{k+1} \left(C_{n-1}^k - C_{N-1}^k a_n^N \right), \quad \text{for} \quad 0 \leqslant n \leqslant N-1, \text{ and } k \geqslant N, \tag{15}$$

since $B_{k+1}/B_k = (k+1)^{-1}$. The convention $C_{-1}^k \equiv 0$ is required, as well as the analogues of the initialization equations (9) and (10), which are

$$C_n^N = B_N a_n^N = \frac{a_n^N}{N!} , \quad \text{for } 0 \leqslant n \leqslant N-1, \tag{16}$$

$$C_n^k = - \frac{\delta_{kn}}{k!} , \qquad \text{for } 0 \leqslant k \leqslant N-1. \tag{17}$$

Note that this method requires explicit computation of the inverse factorials only up to the matrix order N, in contrast to the usage of equation (12b).

The remaining task is the extraction of the coefficients a_n^N from the characteristic polynomial, det $(\lambda I_N - M)$. For a general NxN matrix, there are N^2 coefficients m_{ij} involved, and the task is algebraically complicated. However, for a tri-diagonal matrix M, the coefficients a_n^N may be determined recursively. First note from the determinant

$$p^N(\lambda) = \begin{vmatrix} \lambda - m_{11} & -m_{12} & 0 & 0 & \cdots & \cdots & 0 \\ -m_{21} & \lambda - m_{22} & -m_{23} & 0 & \cdots & \cdots & 0 \\ 0 & -m_{32} & \lambda - m_{33} & -m_{34} & \cdots & \cdots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \cdots & \cdots & -m_{N-1,N-2} & \lambda - m_{N-1,N-1} & & -m_{N-1,N} \\ 0 & \cdots & \cdots & 0 & -m_{N,N-1} & & \lambda - m_{N,N} \end{vmatrix}, \tag{18}$$

the relationship obtained by expanding up the last column:

$$p^N(\lambda) = (\lambda - m_{N,N})\, p^{N-1}(\lambda) - m_{N-1,N}\, m_{N,N-1}\, p^{N-2}(\lambda), \tag{19}$$

where p^{N-1} and p^{N-2} are the appropriate sub-determinants of $p^N(\lambda)$. Substituting the definition (1) in equation (19), we obtain

$$\sum_{n=0}^{N} a_n^N \lambda^n = \sum_{n=1}^{N} a_{n-1}^{N-1} \lambda^n - m_{N,N} \sum_{n=0}^{N-1} a_n^{N-1} \lambda^n - m_{N-1,N}\, m_{N,N-1} \sum_{n=0}^{N-2} a_n^{N-2} \lambda^n . \tag{20}$$

Equating coefficients of like powers of λ on both sides, we obtain the recursion relations:

$$a_N^N = a_{N-1}^{N-1} = 1 \qquad \text{(by definition)}, \tag{21a}$$

$$a_{N-1}^{N} = a_{N-2}^{N-1} - m_{N,N}, \tag{21b}$$

$$a_{n}^{N} = a_{n-1}^{N-1} - m_{N,N}\, a_{n}^{N-1} - m_{N-1,N}\, m_{N,N-1}\, a_{n}^{N-2}, \tag{21c}$$

$$\text{for } 1 \leqslant n \leqslant N-2,$$

$$a_{0}^{N} = -m_{N,N}\, a_{0}^{N-1} - m_{N-1,N}\, m_{N,N-1}\, a_{0}^{N-2} \tag{21d}$$

The recursion relations (21) clearly also hold for any $\overline{N}x\overline{N}$ submatrix of M containing the elements m_{ij} where $1 \leqslant i, j \leqslant \overline{N}$, so that directly we have:

$$p^1(\lambda) = \lambda - m_{11}, \tag{22a}$$

$$p^2(\lambda) = \begin{vmatrix} \lambda - m_{11} & -m_{12} \\ -m_{21} & \lambda - m_{22} \end{vmatrix}$$

$$= \lambda^2 - (m_{11} + m_{22})\lambda + (m_{11}\, m_{22} - m_{12}\, m_{21}). \tag{22b}$$

Since $p^1(\lambda) = a_0^1 + a_1^1 \lambda$ and $p^2(\lambda) = a_0^2 + a_1^2 \lambda + a_2^2 \lambda^2$, it is seen that the initial values for the recursions are

$$a_1^1 = 1; \quad a_0^1 = -m_{11}, \tag{23a}$$

$$a_2^2 = 1; \quad a_1^2 = -(m_{11} + m_{22}); \quad a_0^2 = m_{11}\, m_{22} - m_{12}\, m_{21}. \tag{23b}$$

The coefficients $a_n^{\overline{N}}$ may be generated recursively by using the formulas (21) with N replaced by $\overline{N}$ for $\overline{N} = 3$ to $\overline{N} = N$. Alternatively, equation (19) will generate $p^2(\lambda)$ from $p^1(\lambda)$ and $p^0(\lambda) \equiv 1$, so the recursive technique can actually start with $\overline{N} = 2$.

NUMERICAL EXAMPLE 1: ROTATION RATE MATRIX

As an example, consider the 3x3 infinitesimal rotation rate matrix [2, p. 127], which happens to be skew-symmetric:

$$\omega = \begin{bmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{bmatrix} \tag{24}$$

If we set $\omega_2 = 0$, then ω is a tri-diagonal matrix, and the techniques of the previous section may be applied. The initial values (23) are

$$a_0^1 = -m_{11} = 0 , \tag{25a}$$

$$a_1^2 = -(m_{11} + m_{22}) = 0 , \tag{25b}$$

$$a_0^2 = m_{11}\, m_{22} - m_{12}\, m_{21} = \omega_3^2 , \tag{25c}$$

and the recursion relations (21) yield

$$a_0^3 = -m_{33}\, a_0^2 - m_{23}\, m_{32}\, a_0^1 = 0 , \tag{26a}$$

$$a_1^3 = a_0^2 - m_{33}\, a_1^2 - m_{23}\, m_{32}\, a_1^1 = \omega_3^2 + \omega_1^2 \equiv |\omega|^2 , \tag{26b}$$

$$a_2^3 = a_1^2 - m_{33} = 0 . \tag{26c}$$

Thus, equation (2) becomes

$$\omega^3 = -\sum_{n=0}^{2} a_n^3\, \omega^n = -|\omega|^2\, \omega . \tag{27}$$

At this point, the tri-diagonal restriction (viz., that $\omega_2 = 0$) can be relaxed, since the result (27) also

holds for $\omega_2 \neq 0$, with the generalized definition that $|\omega|^2 \equiv \omega_1^2 + \omega_2^2 + \omega_3^2$, as may be verified by direct calculation. The recursion relations (8) become

$$A_n^{k+1} = A_{n-1}^k - A_2^k |\omega|^2 \delta_{1n}, \quad \text{for } 0 \leqslant n \leqslant 2 \text{ and } k \geqslant 3, \tag{28}$$

since $a_n^3 = |\omega|^2 \delta_{1n}$ for $0 \leqslant n \leqslant 2$ as a result of equations (26). Evaluation of equation (28) produces the following results:

$$A_n^4 = A_{n-1}^3 - A_2^3 |\omega|^2 \delta_{1n} = |\omega|^2 \delta_{2n}, \tag{29a}$$

$$A_n^5 = A_{n-1}^4 - A_2^4 |\omega|^2 \delta_{1n} = -|\omega|^4 \delta_{1n}, \tag{29b}$$

$$A_n^6 = A_{n-1}^5 - A_2^5 |\omega|^2 \delta_{1n} = -|\omega|^4 \delta_{2n}, \tag{29c}$$

$$A_n^7 = A_{n-1}^6 - A_2^6 |\omega|^2 \delta_{1n} = |\omega|^6 \delta_{1n}, \tag{29d}$$

$$A_n^8 = A_{n-1}^7 - A_2^7 |\omega|^2 \delta_{1n} = |\omega|^6 \delta_{2n}. \tag{29e}$$

The above pattern demonstrates that equation (3) becomes

$$\left.\begin{aligned} \omega^{2k+1} &= (-1)^k |\omega|^{2k} \omega \\ \omega^{2k+2} &= (-1)^k |\omega|^{2k} \omega^2 \end{aligned}\right\} \quad \text{for } k = 1, 2, \ldots, \tag{30}$$

where ω^2 is given explicitly as

$$\omega^2 = \begin{bmatrix} -(\omega_2^2 + \omega_3^2) & \omega_1 \omega_2 & \omega_1 \omega_3 \\ \omega_1 \omega_2 & -(\omega_1^2 + \omega_3^2) & \omega_2 \omega_3 \\ \omega_1 \omega_3 & \omega_2 \omega_3 & -(\omega_1^2 + \omega_2^2) \end{bmatrix} \tag{31}$$

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The function

$$f(\omega t) = \sum_{k=0}^{\infty} B_k (\omega t)^k \tag{32}$$

becomes, upon substitution of equation (30),

$$\begin{aligned} f(\omega t) = {} & B_0 I_3 + [\sum_{k=0}^{\infty} B_{2k+1} (-1)^k |\omega|^{2k} t^{2k+1}] \omega \\ & + [\sum_{k=0}^{\infty} B_{2k+2} (-1)^k |\omega|^{2k} t^{2k+2}] \omega^2 . \end{aligned} \tag{33}$$

For the function $f(X) = e^X$ for which $B_k = 1/k!$, this becomes

$$e^{\omega t} = I_3 + \left[\sum_{k=0}^{\infty} \frac{(-|\omega|^2 t^2)^k t}{(2k+1)!} \right] \omega + \left[\sum_{k=0}^{\infty} \frac{(-|\omega|^2 t^2)^k t^2}{(2k+2)!} \right] \omega^2 , \tag{34}$$

or, upon recognition of the bracketed terms as MacLaurin trigonometric series expansions for the sine and cosine,

$$e^{\omega t} = I_3 + \left(\frac{\sin |\omega| t}{|\omega|} \right) \omega + \left(\frac{1 - \cos |\omega| t}{|\omega|^2} \right) \omega^2 . \tag{35}$$

Note that if $|\omega| > 1$, then the calculation of the A_n^k coefficients, as shown in equations (29), produces an unbounded sequence. This may readily be avoided by the use of the recursion (15) and the calculation of the C_n^k coefficients of definition (13) in place of A_n^k, where the sequence of C_n^k converges to zero. Specific numerical values of these coefficients are shown in Table 1, for the rotation rate matrix with $\omega_1 = 1$, $\omega_2 = 0$, and $\omega_3 = 3$.

In the calculation of the infinite summations appearing in equation (14), the relative error in the partial sums after each block of N terms is computed and compared to a pre-selected convergence criterion ϵ in order to evaluate numerically whether convergence has been attained. That is, convergence is deemed to occur when

$$\left| \frac{\sum_{k=0}^{pN-1} C_n^k - \sum_{k=0}^{(p-1)N-1} C_n^k}{\sum_{k=0}^{pN-1} C_n^k} \right| < \epsilon \quad \text{for } 0 \leqslant n \leqslant N-1 \text{ and } p = 2, 3, \ldots \tag{36}$$

Partial sums are compared only after each block of N terms is accumulated into the summation in order to rule out false indications of convergence due to a given term C_n^k vanishing. For a rather stringent convergence criterion of $\epsilon = 10^{-15}$, the summation $\sum_{k=0}^{\infty} C_1^k$ converged after 33 terms ($p = 11$ blocks) to the value $-\sin|\omega|/|\omega| \cong 6.5407 \times 10^{-3}$, and the summation $\sum_{k=0}^{\infty} C_2^k$ converged after 30 terms ($p = 10$ blocks) to the value $-(1-\cos|\omega|)/|\omega|^2 \cong -0.19998$, where $|\omega|^2 = 10$ for the matrix previously cited.

Table 1
Comparison of Selected Values for the Scalar Coefficients
(Rotation Rate Matrix with $\omega_1 = 1, \omega_2 = 0, \omega_3 = 3$)

Indices		Scalar Coefficients	
n	k	A_n^k [eq. (8)]	C_n^k [eq. (15)]
1	1	-1	-1
1	5	-100	-0.833
1	15	10^7	7.65×10^{-6}
1	25	-10^{12}	-6.45×10^{-14}
1	35	10^{17}	9.68×10^{-24}
1	45	-10^{22}	-8.36×10^{-35}
2	2	-1	-0.5
2	6	-100	-0.139
2	10	-10^4	-2.76×10^{-3}
2	20	10^9	4.11×10^{-10}
2	30	-10^{14}	-3.77×10^{-19}
2	40	10^{19}	1.23×10^{-29}

NUMERICAL EXAMPLE 2: FINITE DIFFERENCE MATRIX

As a second example, consider the NxN tri-diagonal and symmetric matrix:

$$T_N = \begin{bmatrix} -2 & 1 & 0 & 0 \cdots 0 & 0 & 0 \\ 1 & -2 & 1 & 0 \cdots 0 & 0 & 0 \\ 0 & 1 & -2 & 1 \cdots 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \quad \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \cdots 1 & -2 & 1 \\ 0 & 0 & 0 & 0 \cdots 0 & 1 & -2 \end{bmatrix}, \qquad (37)$$

where the diagonal entries are all −2 and the super- and sub-diagonal entries are all unity. This matrix arises frequently in the numerical solution of partial differential equations, in particular in the explicit finite difference approximation to the heat conduction equation [3, pp. 60-64]. The eigenvalues of T_N are

$$\lambda_n = -4 \sin^2 \left(\frac{n\pi}{2N+2} \right), \quad \text{for } n = 1, 2, \ldots, N, \qquad (38)$$

and the corresponding eigenvectors are

$$u_n = \left[\sin \frac{n\pi}{N+1}, \sin \frac{2n\pi}{N+1}, \ldots, \sin \frac{Nn\pi}{N+1} \right]^t, \quad \text{for } n = 1, 2, \ldots, N, \qquad (39)$$

where the superscript "t" indicates the transpose. These values can be verified by substitution into $T_N u_n = \lambda_n u_n$.

The initial values (23) are, in this case,

$$a_0^1 = 2; \; a_1^2 = 4; \; a_0^2 = 3, \qquad (40)$$

and the recursion relations (21) yield

$$a_0^N = 2a_0^{N-1} - a_0^{N-2} , \tag{41a}$$

$$a_n^N = a_{n-1}^{N-1} + 2a_n^{N-1} - a_n^{N-2}, \quad \text{for } 1 \leqslant n \leqslant N-2 , \tag{41b}$$

$$a_{N-1}^N = a_{N-2}^{N-1} + 2 , \tag{41c}$$

so that, with N replaced by $\overline{N} = 3$, we find

$$a_0^3 = 2a_0^2 - a_0^1 = 4 , \tag{42a}$$

$$a_1^3 = a_0^2 + 2a_1^2 - a_1^1 = 10 , \tag{42b}$$

$$a_2^3 = a_1^2 + 2 = 6 , \tag{42c}$$

and, with N replaced by $\overline{N} = 4$, we find

$$a_0^4 = 2a_0^3 - a_0^2 = 5 , \tag{43a}$$

$$a_1^4 = a_0^3 + 2a_1^3 - a_1^2 = 20 , \tag{43b}$$

$$a_2^4 = a_1^3 + 2a_2^3 - a_2^2 = 21 , \tag{43c}$$

$$a_3^4 = a_2^3 + 2 = 8 . \tag{43d}$$

This recursion process may be continued, and Table 2 displays the full array of coefficients a_n^N for matrix order N = 8. The final row of Table 2 thus provides the coefficients in the characteristic polynomial $p^8(\lambda)$ of equation (1), as well as the coefficients of each of the powers $I_8, T_8, T_8^2, \ldots,$ T_8^7 appearing in the summation of equation (2). Upon calculation, each of the sequences C_n^k for $n = 0, 1, 2, \ldots, 7$ of equation (15) is seen to converge toward zero as $k \rightarrow \infty$. In the calculation of the infinite summations appearing in equation (14), convergence is based on the inequality (36) for

Table 2

Full Array of Coefficients a_n^N
(Finite Difference Matrix of Order N = 8)

Index N \ n	0	1	2	3	4	5	6	7	8
0	1								
1	2	1							
2	3	4	1						
3	4	10	6	1					
4	5	20	21	8	1				
5	6	35	56	36	10	1			
6	7	56	126	120	55	12	1		
7	8	84	252	330	220	78	14	1	
8	9	120	462	792	715	364	105	16	1

(Header spanning columns n = 0–8: Value of Coefficients a_n^N)

the same criterion of $\epsilon = 10^{-15}$ as used in the previous example. Results of applying this convergence criterion are shown in Table 3. It is noted that convergence in all 8 summations is attained

Table 3

Convergence Properties of the Summations $\sum_{k=0}^{\infty} C_n^k$
(Finite Difference Matrix of Order N = 8 with Criterion $\epsilon = 10^{-15}$)

Summation n	Convergence after		Approximate Summation Value
	k terms	p blocks	
0	40	5	−0.99996
1	40	5	−0.99944
2	40	5	−0.49779
3	40	5	−0.16272
4	48	6	-3.7853×10^{-2}
5	48	6	-6.1599×10^{-3}
6	48	6	-6.2691×10^{-4}
7	48	6	-2.9581×10^{-5}

after either 5 or 6 blocks of 8 terms each and that the converged absolute values of the summations monotonically decrease with the power of T_8 with which they are associated in equation (14).

The quantity $\exp(T_N)$ may be computed numerically by equation (14). With the known eigenvalues (38) and eigenvectors (39) of T_N, the exponential matrix may readily be determined analytically as well. Since the N eigenvalues of T_N are distinct, T_N is similar to a diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$ whose entries are the eigenvalues of T_N [1, p. 77], or

$$T_N = S \Lambda S^{-1} , \tag{44}$$

where the similarity transformation matrix S is formed of ordered columns composed of the eigenvectors of T_N. Furthermore, since T_N is symmetric, its eigenvectors are mutually orthogonal [1, p. 99]. If, in addition, the eigenvectors (39) are normalized, so that $u_n' \equiv u_n/|u_n|$, then the similarity matrix S' formed of ordered columns composed of the u_n' vectors will be a unitary matrix such that $(S')^{-1} = (S')^t$. By the "telescoping" property of the similarity transformation, for any positive integer k,

$$\begin{aligned} T_N^k &= (S\Lambda S^{-1})^k = (S\Lambda S^{-1})(S\Lambda S^{-1}) \ldots (S\Lambda S^{-1}) \text{ for k factors} \\ &= S\Lambda^k S^{-1} , \end{aligned} \tag{45}$$

so that

$$\begin{aligned} \exp(T_N) &\equiv \sum_{k=0}^{\infty} \frac{T_N^k}{k!} = \sum_{k=0}^{\infty} \frac{S\Lambda^k S^{-1}}{k!} = S\left(\sum_{k=0}^{\infty} \frac{\Lambda^k}{k!}\right) S^{-1} \\ &= S\,[\exp(\Lambda)]\, S^{-1} . \end{aligned} \tag{46}$$

Since Λ is a diagonal matrix, $\Lambda^k = \mathrm{diag}(\lambda_1^k, \lambda_2^k, \ldots, \lambda_N^k)$, and $\exp(\Lambda) = \mathrm{diag}(e^{\lambda_1}, e^{\lambda_2}, \ldots, e^{\lambda_N})$. If, in equation (46), S' is substituted for S, then the final result is

$$\exp(T_N) = S' [\mathrm{diag}(e^{\lambda_1}, e^{\lambda_2}, \ldots, e^{\lambda_N})] (S')^t . \tag{47}$$

For the value N = 8, Table 4 presents the eigenvalues (38) and unnormalized eigenvectors (39) of T_N, where, due to the periodic properties of the sine function, there are only four non-zero magnitudes involved in the 64 eigenvector components. Note that the eigenvalues span more than an

Table 4

Eigenvalues and Unnormalized Eigenvectors
(Finite Difference Matrix of Order N = 8)

Eigenvalues λ_n [Eq. (38)]	Eigenvector Components* [Eq. (39)]							
	u_1	u_2	u_3	u_4	u_5	u_6	u_7	u_8
$\lambda_1 = -0.12061476$	s_1	s_2	s_3	s_4	s_4	s_3	s_2	s_1
$\lambda_2 = -0.46791111$	s_2	s_4	s_3	s_1	$-s_1$	$-s_3$	$-s_4$	$-s_2$
$\lambda_3 = -1$	s_3	s_3	0	$-s_3$	$-s_3$	0	s_3	s_3
$\lambda_4 = -1.65270365$	s_4	s_1	$-s_3$	$-s_2$	s_2	s_3	$-s_1$	$-s_4$
$\lambda_5 = -2.34729636$	s_4	$-s_1$	$-s_3$	s_2	s_2	$-s_3$	$-s_1$	s_4
$\lambda_6 = -3$	s_3	$-s_3$	0	s_3	$-s_3$	0	s_3	$-s_3$
$\lambda_7 = -3.53208889$	s_2	$-s_4$	s_3	$-s_1$	$-s_1$	s_3	$-s_4$	s_2
$\lambda_8 = -3.87938524$	s_1	$-s_2$	s_3	$-s_4$	s_4	$-s_3$	s_2	$-s_1$

*where, by definition,

$$s_1 \equiv \sin \pi/9 = 0.34202014,$$
$$s_2 \equiv \sin 2\pi/9 = 0.64278761,$$
$$s_3 \equiv \sin \pi/3 = \sqrt{3}/2 = 0.86602540,$$
$$s_4 \equiv \sin 4\pi/9 = 0.98480775.$$

order of magnitude, since the maximum ratio is $\lambda_8/\lambda_1 \cong 32$. Since the eigenvectors are all of magnitude $|u|^2 = |u_n|^2 = 9/2$ for $n = 1, 2, \ldots, 8$, the normalized similarity transformation matrix S′ is given explicitly by

$$S' = \frac{\sqrt{2}}{3}\begin{bmatrix} s_1 & s_2 & s_3 & s_4 & s_4 & s_3 & s_2 & s_1 \\ s_2 & s_4 & s_3 & s_1 & -s_1 & -s_3 & -s_4 & -s_2 \\ s_3 & s_3 & 0 & -s_3 & -s_3 & 0 & s_3 & s_3 \\ s_4 & s_1 & -s_3 & -s_2 & s_2 & s_3 & -s_1 & -s_4 \\ s_4 & -s_1 & -s_3 & s_2 & s_2 & -s_3 & -s_1 & s_4 \\ s_3 & -s_3 & 0 & s_3 & -s_3 & 0 & s_3 & -s_3 \\ s_2 & -s_4 & s_3 & -s_1 & -s_1 & s_3 & -s_4 & s_2 \\ s_1 & -s_2 & s_3 & -s_4 & s_4 & -s_3 & s_2 & -s_1 \end{bmatrix}, \qquad (48)$$

where $s_1 \equiv \sin \pi/9$, $s_2 \equiv \sin 2\pi/9$, $s_3 \equiv \sin \pi/3 = \sqrt{3}/2$, and $s_4 \equiv \sin 4\pi/9$. Note that S′ is symmetric as well as unitary, so that $(S')^t = (S')^{-1} = S'$. On inserting equation (48) into equation (47), it is found that $\exp(T_8)$ is both symmetrical and "back-symmetrical"; that is, the exponential matrix exhibits symmetry about both principal diagonals. Explicitly, the exponential matrix is of the form

$$\exp(T_8) = \begin{bmatrix} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 & e_7 & e_8 \\ e_2 & e_9 & e_{10} & e_{11} & e_{12} & e_{13} & e_{14} & e_7 \\ e_3 & e_{10} & e_{15} & e_{16} & e_{17} & e_{18} & e_{13} & e_6 \\ e_4 & e_{11} & e_{16} & e_{19} & e_{20} & e_{17} & e_{12} & e_5 \\ e_5 & e_{12} & e_{17} & e_{20} & e_{19} & e_{16} & e_{11} & e_4 \\ e_6 & e_{13} & e_{18} & e_{17} & e_{16} & e_{15} & e_{10} & e_3 \\ e_7 & e_{14} & e_{13} & e_{12} & e_{11} & e_{10} & e_9 & e_2 \\ e_8 & e_7 & e_6 & e_5 & e_4 & e_3 & e_2 & e_1 \end{bmatrix}, \qquad (49)$$

where both the analytical and numerical values for each of the 20 distinct elements e_i are given in Table 5.

Table 5

Analytical and Numerical Values for Exponential Matrix Elements
(Finite Difference Matrix of Order N = 8)

Symbol	Analytical Expression*	Numerical Value
e_1	$s_1^2 E_{18}^+ + s_2^2 E_{27}^+ + s_3^2 E_{36}^+ + s_4^2 E_{45}^+$	0.21526929
e_2	$s_1 s_2 E_{18}^- + s_2 s_4 E_{27}^- + s_3^2 E_{36}^- + s_1 s_4 E_{45}^-$	0.18647807
e_3	$s_1 s_3 E_{18}^+ + s_2 s_3 E_{27}^+ - s_3 s_4 E_{45}^+$	$8.63736679 \times 10^{-2}$
e_4	$s_1 s_4 E_{18}^- + s_1 s_2 E_{27}^- - s_3^2 E_{36}^- - s_2 s_4 E_{45}^-$	$2.74614615 \times 10^{-2}$
e_5	$s_1 s_4 E_{18}^+ - s_1 s_2 E_{27}^+ - s_3^2 E_{36}^+ + s_2 s_4 E_{45}^+$	$6.64880517 \times 10^{-3}$
e_6	$s_1 s_3 E_{18}^- - s_2 s_3 E_{27}^- + s_3 s_4 E_{45}^-$	$1.29935583 \times 10^{-3}$
e_7	$s_1 s_2 E_{18}^+ - s_2 s_4 E_{27}^+ + s_3^2 E_{36}^+ - s_1 s_4 E_{45}^+$	$2.12770688 \times 10^{-4}$
e_8	$s_1^2 E_{18}^- - s_2^2 E_{27}^- + s_3^2 E_{36}^- - s_4^2 E_{45}^-$	$2.95813145 \times 10^{-5}$
e_9	$s_2^2 E_{18}^+ + s_4^2 E_{27}^+ + s_3^2 E_{36}^+ + s_1^2 E_{45}^+$	0.30164296
e_{10}	$s_2 s_3 E_{18}^- + s_3 s_4 E_{27}^- - s_1 s_3 E_{45}^-$	0.21393953
e_{11}	$s_2 s_4 E_{18}^+ + s_1 s_4 E_{27}^+ - s_3^2 E_{36}^+ - s_1 s_2 E_{45}^+$	$9.30224731 \times 10^{-2}$
e_{12}	$s_2 s_4 E_{18}^- - s_1 s_4 E_{27}^- - s_3^2 E_{36}^- + s_1 s_2 E_{45}^-$	$2.87608174 \times 10^{-2}$
e_{13}	$s_2 s_3 E_{18}^+ - s_3 s_4 E_{27}^+ + s_1 s_3 E_{45}^+$	$6.86157586 \times 10^{-3}$
e_{14}	$s_2^2 E_{18}^- - s_4^2 E_{27}^- + s_3^2 E_{36}^- - s_1^2 E_{45}^-$	$1.32893715 \times 10^{-3}$
e_{15}	$s_3^2 (E_{18}^+ + E_{27}^+ + E_{45}^+)$	0.30829176
e_{16}	$s_3 s_4 E_{18}^- + s_1 s_3 E_{27}^- + s_2 s_3 E_{45}^-$	0.21523888
e_{17}	$s_3 s_4 E_{18}^+ - s_1 s_3 E_{27}^+ - s_2 s_3 E_{45}^+$	$9.32352438 \times 10^{-2}$
e_{18}	$s_3^2 (E_{18}^- - E_{27}^- - E_{45}^-)$	$2.87903987 \times 10^{-2}$
e_{19}	$s_4^2 E_{18}^+ + s_1^2 E_{27}^+ + s_3^2 E_{36}^+ + s_2^2 E_{45}^+$	0.30850453
e_{20}	$s_4^2 E_{18}^- - s_1^2 E_{27}^- + s_3^2 E_{36}^- - s_2^2 E_{45}^-$	0.21526847

*where, by definition, $E_{18}^{\pm} \equiv e^{\lambda_1} \pm e^{\lambda_8}$, $E_{27}^{\pm} \equiv e^{\lambda_2} \pm e^{\lambda_7}$,

$E_{36}^{\pm} \equiv e^{\lambda_3} \pm e^{\lambda_6}$, $E_{45}^{\pm} \equiv e^{\lambda_4} \pm e^{\lambda_5}$.

The convergence properties of the infinite summations $\sum_{k=0}^{\infty} C_n^k$ appearing in equation (14) were further investigated for finite difference matrices of orders N = 2, 4, 6, 8, and 10. The results are summarized in Table 6 for the convergence criterion $\epsilon = 10^{-15}$ used earlier as well as for a more relaxed criterion of $\epsilon = 10^{-10}$. It is seen that use of the more stringent criterion leads to a modest

Table 6

Convergence Properties* of the Summations $\sum_{k=0}^{\infty} C_n^k$ for Finite Difference Matrix of Order N

A. Using Criterion $\epsilon = 10^{-10}$

Summation, n / Matrix Order, N	Number of terms, k required for convergence									
N \ n	0	1	2	3	4	5	6	7	8	9
2	24	24								
4	28	28	28	32						
6	30	30	36	36	36	36				
8	32	32	40	40	40	40	40	40		
10	40	40	40	40	40	40	40	40	40	40

B. Using Criterion $\epsilon = 10^{-15}$

Summation, n / Matrix Order, N	Number of terms, k required for convergence									
N \ n	0	1	2	3	4	5	6	7	8	9
2	30	30								
4	36	36	36	36						
6	36	36	42	42	42	42				
8	40	40	40	40	48	48	48	48		
10	40	40	50	50	50	50	50	50	50	50

*The number of blocks, p required for convergence is given by p = k/N.

increase in the number of terms required for convergence. Note also that the number, $p = k/N$ of blocks required for convergence actually decreases as the matrix order N increases: for $N = 2$, $p = 12$ or 15; for $N = 4$, $p = 7, 8$, or 9; for $N = 6$, $p = 5, 6$, or 7; for $N = 8$, $p = 4, 5$, or 6; and for $N = 10$, $p = 4$ or 5. The summations denoted by the lower integer values n converge to larger absolute values than those denoted by larger values of n (see Table 3), and the former converge more rapidly, viz., generally, convergence is attained one block earlier. The most significant result indicated by Table 6, however, is that as the order N of the matrix increases, the number k of terms required for convergence of the infinite summations increases very slowly.

A final investigation was made into the properties of the exponential matrix raised to an integral power. Specifically, calculations were made to evaluate the matrices $(\exp T_N)^\ell$, where the exponent ℓ is itself a positive integral power of two. Table 7 presents the range of matrix elements for the matrices $(\exp T_8)^\ell$, where $\ell = 2^q$, for $q = 0, 1, \ldots, 9$. These matrices are readily evaluated

Table 7

Range* of Elements for Successive Squarings of Exponential Matrix of Order N = 8

Value of Power, ℓ	Minimum Element of Matrix $(\exp T_8)^\ell$	Maximum Element of Matrix $(\exp T_8)^\ell$
1	2.96×10^{-5}	3.09×10^{-1}
2	6.82×10^{-4}	2.07×10^{-1}
4	4.70×10^{-3}	1.40×10^{-1}
8	7.79×10^{-3}	8.28×10^{-2}
16	3.72×10^{-3}	3.13×10^{-2}
32	5.48×10^{-4}	4.54×10^{-3}
64	1.15×10^{-5}	9.57×10^{-5}
128	5.13×10^{-9}	4.25×10^{-8}
256	1.01×10^{-15}	8.39×10^{-15}
512	3.94×10^{-29}	3.26×10^{-28}

*All elements of all matrices are positive.

by successive squarings of the form $(\exp T_8)^{2^q} = (\exp T_8)^{2^{q-1}} (\exp T_8)^{2^{q-1}}$, so that for $\ell = 2^q$, only q successive matrix squarings are necessary. An analytical check is readily at hand, since by the "telescoping" property of the similarity transformation, both sides of equation (47) can be raised to the power ℓ as

$$[\exp(T_N)]^{\ell} = S' [\mathrm{diag}(e^{\ell\lambda_1}, e^{\ell\lambda_2}, \ldots, e^{\ell\lambda_N})] (S')^t. \tag{50}$$

Table 7 shows that as ℓ increases, the maximum element of $(\exp T_8)^{\ell}$ monotonically decreases. The minimum element of $(\exp T_8)^{\ell}$ initially increases with ℓ, but then later also decreases as ℓ increases. Most significantly, the range of elements within the matrix $(\exp T_8)^{\ell}$ monotonically decreases as ℓ increases and $(\exp T_8)^{\ell}$ approaches the zero matrix as $\ell \to \infty$ in a rather smooth fashion. The smoothness of the convergence toward zero, and the decreases in the range of the matrix elements, are due to the dominance of the largest eigenvalue, λ_1 (refer to Table 4).

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APPENDIX

ALGORITHM FOR EVALUATION OF EXPONENTIAL MATRICES

1. The following parameters are given initially:

   a. the matrix order N, where $N \geqslant 2$ is a positive integer;

   b. the upper limit, N_{max}, on the number of recursions calculated, where $N_{max} \gg N$ is a positive integer;

   c. the criterion, ϵ, for convergence of the partial sums, where $0 < \epsilon \ll 1$; and

   d. the tri-diagonal square matrix M of order N. This can be efficiently provided by initializing M as an N x N zero matrix and then substituting the elements on the principal diagonal, the super-diagonal, and the sub-diagonal, as follows:

   $m_{i,i}$ for $i = 1, 2, \ldots, N$,

   $m_{i,i+1}$ for $i = 1, 2, \ldots, N-1$,

   $m_{i+1,i}$ for $i = 1, 2, \ldots, N-1$.

2. The initial values for the array $a_n^{\bar{N}}$ are:

$$a_0^1 = -m_{11}$$

$$a_0^2 = m_{11}\, m_{22} - m_{12}\, m_{21} \qquad (23)^*$$

$$a_1^2 = -m_{11} - m_{22}$$

$$a_n^n = 1 \quad \text{for} \quad n = 0, 1, \ldots, N \qquad (21a)$$

3. The array values $a_n^{\bar{N}}$ are calculated recursively for $\bar{N} = 3, 4, \ldots, N$ from:

$$a_0^{\bar{N}} = -m_{\bar{N},\bar{N}}\, a_0^{\bar{N}-1} - m_{\bar{N}-1,\bar{N}}\, m_{\bar{N},\bar{N}-1}\, a_0^{\bar{N}-2}$$

$$a_n^{\bar{N}} = a_{n-1}^{\bar{N}-1} - m_{\bar{N},\bar{N}}\, a_n^{\bar{N}-1} - m_{\bar{N}-1,\bar{N}}\, m_{\bar{N},\bar{N}-1}\, a_n^{\bar{N}-2} \quad \text{for } n = 1, 2, \ldots, \bar{N}-2 \qquad (21)$$

$$a_{\bar{N}-1}^{\bar{N}} = a_{\bar{N}-2}^{\bar{N}-1} - m_{\bar{N},\bar{N}}$$

*These equation numbers provide a reference to the discussion in the main body of the text.

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4. The initial values for the array C_n^k are:

$$C_n^N = \frac{a_n^N}{N!} \quad \text{for} \quad n = 0, 1, \ldots, N-1 \tag{16}$$

$$\left.\begin{aligned} C_n^k &= 0 \text{ if } k \neq n \\ C_n^k &= -1/k! \text{ if } k = n \end{aligned}\right\} \quad \text{for } n, k = 0, 1, \ldots, N-1 \tag{17}$$

5. The array values C_n^k are calculated recursively for $k = N, N+1, \ldots, N_{max}$ from:

$$C_0^{k+1} = -\frac{C_{N-1}^k a_0^N}{k+1}$$

$$C_n^{k+1} = \frac{1}{k+1}\left(C_{n-1}^k - C_{N-1}^k a_n^N\right) \quad \text{for } n = 1, 2, \ldots, N-1 \tag{15}$$

6. Evaluate integral powers of the tri-diagonal matrix M iteratively, as follows:

$M^0 \equiv I_N$, the NxN identity matrix,

$M^1 \equiv M$,

and $M^k = M^{k-1} M$ for $k = 2, 3, \ldots, N-1$,

or, in terms of matrix elements:

$$m_{ij}^k = \sum_{\ell=1}^{N} m_{i\ell}^{k-1} m_{\ell j}$$

7. Calculate successive partial sum approximations to the infinite sums $\sum_{k=0}^{\infty} C_n^k$ for $n = 0, 1, \ldots,$ $N-1$, and compare the relative differences in successive partial summations after each block of N terms to the convergence criterion, where

$$\left| \frac{\sum_{k=0}^{(p+1)N-1} C_n^k - \sum_{k=0}^{pN-1} C_n^k}{\sum_{k=0}^{(p+1)N-1} C_n^k} \right| < \epsilon \quad \text{for } n = 0, 1, \ldots, N-1 \tag{36}$$

indicates convergence of the summation for some value, $p = 0, 1, \ldots$ (By convention, define $\sum_{k=0}^{pN-1} C_n^k \equiv 0$ for $p = 0$.)

If the above inequality is not satisfied for all zero and positive integral values of p such that $(p+1)N - 1 \leq N_{max}$, then convergence of the infinite sum has not been attained and either N_{max} or ϵ must be increased.

8. The exponential matrix is evaluated as a linear combination of N matrices, as follows:

$$e^M = \sum_{n=0}^{N-1} \left(\sum_{k=0}^{\infty} C_n^k \right) M^n. \tag{14}$$

Note: The above algorithm for the evaluation of exponential matrices has been implemented as a FORTRAN language computer program and is available, upon request, from the authors.